

The Calculation of Molecular Opacities

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The theoretical modeling of the properties and emergent spectra of extra solar giant planets and brown dwarfs requires an accurate and detailed knowledge of the sources of molecular opacity in these objects. In the past few years, many new extra solar planets and brown dwarfs have been discovered using new observational techniques and better, larger telescopes. In order to better understand the physical properties of these new objects and to relate their properties to the properties of other solar systems, astronomers have been using computer-generated models to reproduce their observed properties. This scenario allows a direct comparison between theory and observations and helps to constrain physical properties such as mass, radius, and chemical composition. These objects span the range between the gas giants of our own solar system (Jupiter) and objects almost large enough to burn hydrogen in their interior and thus become stars (brown dwarfs). An accurate theoretical model requires a thorough knowledge of the molecular opacities of a large number of different species, because the temperature in the atmospheres of these objects spans a range from 100 kelvin up to several thousand degrees. Because of the wide range of physical conditions encountered, modelers need molecular opacities up to a range of temperatures that go far beyond the normal range of molecular data from laboratory studies. The purpose of this research is to extend the range of available molecular opacities up to the higher temperatures needed by the modelers.

This extension has been accomplished by using a combination of theoretical techniques combined with available observational data to predict lines of various molecules such as CH₄, VO, and CrH. As an example of what has been accomplished, consider the cases of CH₄, H₂O, and TiO: (methane, water, and titanium oxide). The list of spectral lines was extended for all these species to include lines that will become important at higher temperatures, even though these lines are practically unobservable at room temperatures. Water and methane, in particular, are very important sources of opacity in these objects, and the inclusion of adequate opacity is very

important to properly evaluate their spectra and construct physically realistic models.

In doing this work, the researcher made use of the work of other Ames researchers, especially the work of David Schwenke of the Computational Chemistry Branch. Comparison with observations shows that more work remains to be done to provide opacities that are physically realistic at the highest temperatures, especially for methane and (less so for) water. Even so, the latest models for objects such as the brown dwarf Gl229B (Gliese 229B) show good agreement with the best available observations.

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Mars Atmosphere and Climate

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Furthering our understanding of the global atmospheric circulation on Mars is the focus of this research at Ames Research Center. As in Earth's atmosphere, Mars' atmospheric circulation exhibits variability over a vast range of spatial and temporal scales. Some of these processes are driven by similar physical processes (for example, Hadley circulation cells; global-scale thermal tidal modes; planetary waves forced via flow over large-scale orographic complexes like Earth's Himalayan plateau; and developing, traveling, and decaying extratropical weather cyclones associated with pole-to-equator thermal contrasts). Other sources of variability arise from distinctly Martian physical mechanisms (for example, condensation (sublimation) during the winter (summer) season of the primary chemical constituent of the atmosphere (predominantly carbon dioxide (CO₂), and regional- and global-scale dust storms). Ultimately, these investigations aspire to improve our knowledge of the dynamics of the planet's present environment and past climates, and from a comparative planetology perspective, to better